# ON THE EXTENSION OF THE ANALYTIC NODAL DIFFUSION SOLVER ANDES TO SODIUM FAST REACTORS

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## ABSTRACT

Within the framework of the Collaborative Project for a European Sodium Fast Reactor, the reactor physics group at UPM is working on the extension of its in-house multi-scale advanced deterministic code COBAYA3 to Sodium Fast Reactors (SFR). COBAYA3 is a 3D multigroup neutron kinetics diffusion code that can be used either as a pin-by-pin code or as a stand-alone nodal code by using the analytic nodal diffusion solver ANDES. It is coupled with thermal-hydraulics codes such as COBRA-TF and FLICA, allowing transient analysis of LWR at both fine-mesh and coarse-mesh scales.

In order to enable also 3D pin-by-pin and nodal coupled NK-TH simulations of SFR, different developments are in progress. This paper presents the first steps towards the application of COBAYA3 to this type of reactors. ANDES solver, already extended to triangular-Z geometry, has been applied to fast reactor steady-state calculations. The required cross section libraries were generated with ERANOS code for several configurations. The limitations encountered in the application of the Analytic Coarse Mesh Finite Difference (ACMFD) method –implemented inside ANDES– to fast reactors are presented and the sensitivity of the method when using a high number of energy groups is studied.

ANDES performance is assessed by comparison with the results provided by ERANOS, using a mini-core model in 33 energy groups. Furthermore, a benchmark from the NEA for a small 3D FBR in hexagonal-Z geometry and 4 energy groups is also employed to verify the behavior of the code with few energy groups.

*Key Words*: fast reactors, hexagonal geometry, ACMFD, coarse mesh scale.

## 1. INTRODUCTION

There is an increasing demand on simulation codes for core physics and safety analysis of new reactor technologies, such as the ones considered within the frame of the GEN-IV International Forum. The current codes considered in the state-of-the-art regard only a certain domain of application and are either not coupled together or qualified and tested for advanced fast spectrum systems. Besides, a new trend to unify the codes in a unique system for the analysis of a broad range of hypothetical scenarios for Gen-IV fast reactors has been carried out in Europe.

Following this motivation, the Paul Scherrer Institute (PSI) launched recently (2003) the FAST (Fast-spectrum Advanced Systems for power production and resource managemenT) project [1] in the area of fast spectrum core and safety analysis.

During the last years, the reactor physics group at UPM has been working in the development of in-house multi-discipline advanced deterministic codes to perform 3D core calculations of present and future PWR, BWR and VVER reactors, including efficient neutron kinetics (NK) modules and coupling with thermal-hydraulic (TH) codes for transient analysis. Our 3D multigroup neutron kinetics code is COBAYA3 [2]. It solves the steady-state and time-dependent multi-group neutron diffusion equation for both Cartesian rectangular and triangular-Z geometry, and can be used either as a pin-by-pin code [3] or as a stand-alone nodal code by using the Analytic Nodal Diffusion Solver ANDES [4].

At UPM, we aim to extend our in-house code system to Sodium Fast Reactors in order to enable accurate pin-by-pin (hexagonal cells) and nodal (triangular nodes) coupled NK-TH simulations for this type of reactors. Thus, several objectives have been settled. First, in this paper, we focus on the extension of the 3D multi-group ANDES solver implemented in COBAYA3 code to perform nodal steady-state fast reactor calculations. Interface discontinuity factors will be used to enhance diffusion results in such a way that fast reactor whole core calculations will fit much better detailed transport solutions. Otherwise, the strong flux variations observed in fast reactors could not suitably be taken into account by mere diffusion theory. Then, we will focus on neutron kinetics problems along with thermal-hydraulic coupling for transient analysis. Furthermore, burn-up capabilities will be implemented in ANDES code and finally, an extended Verification & Validation of the performance of ANDES will be carried out for both steady-state and transient calculations.

In Section 2, a description of the Analytic Coarse-Mesh Finite-Difference (ACMFD) method implemented in ANDES is given. Then, in Section 3, we resort to the broad-validated code system for fast reactor calculations ERANOS [5] for cross section generation. Section 4 is devoted to the analysis of ANDES performance for fast reactors, discussing several encountered problems and presenting methodologies implemented in order to overcome them. Some numerical results are presented in Section 5; first, a 3D mini-core previously calculated with ERANOS is used as a home-made benchmark; second, a NEA benchmark for a small 3D FBR in 4 energy groups is selected. Finally, conclusions are presented in Section 6.

## 2. DESCRIPTION OF ANDES SOLVER

The multigroup neutron diffusion solver ANDES is based on the ACMFD (Analytic Coarse-Mesh Finite-Difference) method and is able to perform both 3D kinetics and steady-state nodal calculations for both Cartesian rectangular and triangular-Z geometries. It has been broadly validated with several NEA benchmarks for both PWR and VVER reactors, obtaining highly satisfactory results [4].

### 2.1. Overview of the ACMFD method

The ACMFD method, developed by Y.A. Chao [6], was first fully generalized to multigroup [7] and multidimensional [8] problems and implemented in the ANDES solver for PWR core

analysis. Then, following the same guidelines, the ACMFD methodology was extended to Triangular-Z geometry to be applied to VVER reactors [9]. Excellent performances have been proved in both rectangular and hexagonal geometries, which can be considered as a promising starting point for its application to Gen IV advanced core designs that use hexagonal fuel assembly configurations, such as Sodium Fast Reactors.

The ACMFD method in Cartesian geometry is based on two steps aimed to obtain an analytical solution of the multigroup diffusion equation within homogeneous nodes. The first one is the decoupling of the multigroup diffusion equation by means of diagonalization of the multigroup diffusion matrix **A**, in such a way that we obtain a set of uncoupled diffusion equations over the modal fluxes which are linearly related to the physical fluxes. The second step consists in performing a transverse integration, to reduce the *n*-dimensional diffusion equation into *n* one-dimensional equations, coupled through the transverse leakage included as an external source term.

$$\nabla^2 \,|\, \phi(r)\rangle - A \,|\, \phi(r)\rangle = -D^{-1} \,|\, S(r)\rangle \tag{1}$$

$$A \,|\, u_m\rangle = \lambda_m \,|\, u_m\rangle \;\; ; \quad R^{-1} = [u_m] \;\; ; \quad A = R^{-1}[\lambda_m]_{diag} R \tag{2}$$

Where $\lambda_m$ and $u_m$ are the eigenvalue and eigenvector for mode m. Thus, pre-multiplying equation (1) by matrix **R** and considering that:

$$|\psi_m\rangle = R \,|\, \phi_g\rangle \;\; ; \qquad |\phi_g\rangle = R^{-1} \,|\, \psi_m\rangle \;\; ; \qquad |s_m\rangle = RD^{-1} \,|\, S_g\rangle \;\; ; \quad |S_g\rangle = DR^{-1} \,|\, s_m\rangle \tag{3}$$

The G multigroup coupled equations (1) are reduced to another G uncoupled modal equations which analytical solution is affordable (4).

$$\nabla^2 \psi_m(r) - \lambda_m \psi_m(r) = -s_m(r) \;\; ; \qquad m = 1, G \tag{4}$$

While the first step is independent of the geometry and only related to the material properties of each node represented by its cross sections; the second step, i.e. the transverse leakage integration procedure, required additional developments when extended to triangular-Z geometry [9]. Triangular nodes instead of hexagonal ones were preferred in order to avoid the singularities that appear when applying transverse integration to hexagonal nodes, allowing moreover the advantage of the mesh subdivision capabilities implicit within that geometry.

Interface discontinuity factors can be easily introduced in the ACMFD method. In this way, flux distribution would be modified from that obtained in coarse homogenized regions, making diffusion solutions much more accurate.

## 3. ERANOS CODE

### 3.1. Description of ERANOS code system

ERANOS is a deterministic code system that performs core, shielding, as well as fuel cycle calculations, and includes the most recent developments in calculational methods, such as the collision probability method in many groups and a 3D nodal transport theory variational method with perturbation theory and kinetics options.

ERANOS calculations require ECCO results; ECCO is a cell code based on the sub-group method combined with a fine group transport calculation to compute homogenized cross sections considering the isotopic composition of each cell. ECCO can solve either homogeneous descriptions of assemblies and pins, or heterogeneous ones including the detailed geometry.

These macroscopic cross sections can then be used in the ERANOS code to model the entire core and to solve the diffusion or the transport equation in RZ or 3D geometries. With the neutron flux already calculated, the user can do a depletion calculation solving Bateman equations. Once the new isotopic concentrations have been calculated, macroscopic cross sections can be directly updated to do a new core calculation, or a new ECCO cell calculation to update the macroscopic cross sections can be performed.

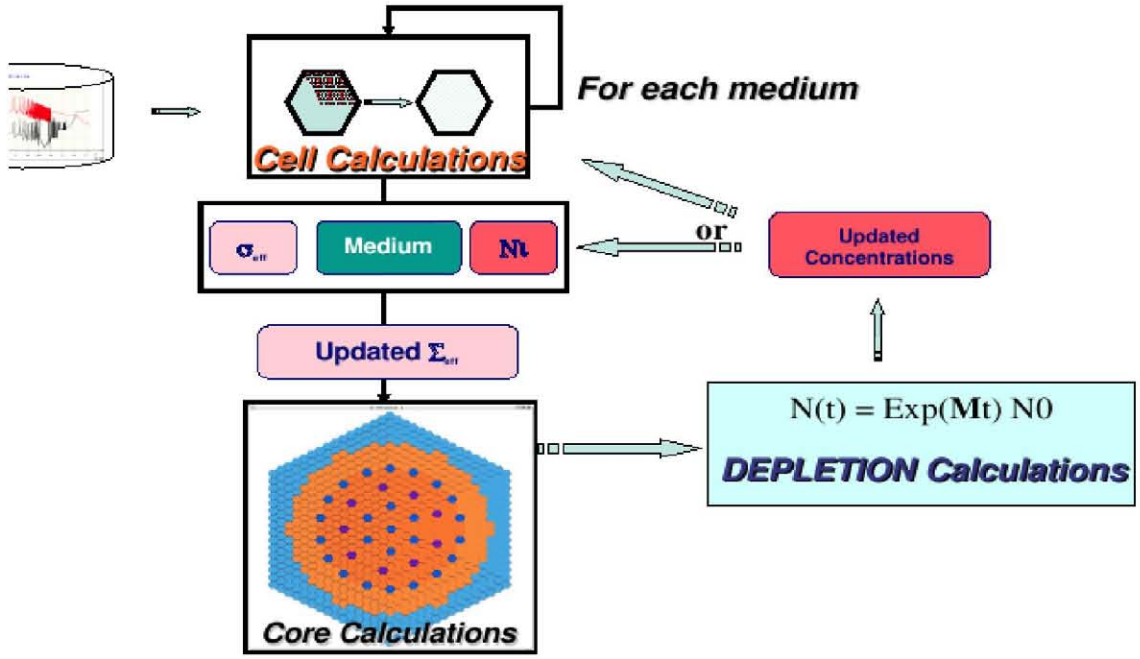


**Figure 1. Description of ERANOS system**

The first option is usually adopted as it is a good approximation for fast reactors to assume that microscopic cross sections calculated for every group of energy will not change much, reducing

the calculation time. This core calculation employing ERANOS/ECCO system is described in Fig.1.

For RZ models of the core, both transport and diffusion equations can be solved employing BISTRO solver. For a 3D model (Cartesian or Hexagonal-Z), the diffusion equation will be solved with H3D solver and the transport equation with VARIANT solver. The advantage of employing BISTRO solver is that it will provide a high capacity of space discretization and perturbation studies.

Depending on both the type of calculation required and the library used, the ECCO computation can be done with 33, 172, 175 or 1968 energy groups. Most of the time, it is sufficient to do a 1968 group calculation for the self shielding calculation condensed to 33 groups. The ERANOS flux calculation can only be done with 33 groups in transport because of computer memory shortages, while the diffusion equation could be solved with a 172 energy group discretization.

### 3.2. Cross section generation

Before running ANDES code, it is necessary to have at our disposal a tabularized cross section library which had to be either generated by a transport code for a defined configuration or provided by a benchmark specification. In our case, ERANOS was chosen as the transport code to obtain the cross sections because of its widely validated results.

Full core fast reactor calculations require a finer energy group structure than thermal reactor calculations. In fact, no less than 33 groups are recommendable, so that a calculation using ECCO module was performed in this number of energy groups using the cell description of the subassemblies presented in the European Sodium Fast Reactor (ESFR) core [10].

**Table I. Overview of cross sections and other parameters of the library for diffusion non-kinetics calculations.**

| Quantity | Unit |
|---|---|
| Diffusion coefficient | cm |
| Absorption cross section | 1/cm |
| Fission neutron-production cross section | 1/cm |
| Fission energy-production cross section | Ws/cm |
| P0-Scattering matrix (Multi-group diffusion) | 1/cm |
| Fission spectrum | 1 |

All the tabularized parameters required by ANDES, shown in Table I, were successfully generated by ERANOS code for every heterogeneous assembly described in ESFR core specification, and extracted from the output to create the cross sections library to be provided to ANDES.

## 4. APPLICATION OF ANDES CODE TO SFR

Several considerations linked to fast reactor calculations with respect to thermal reactor's, such as the finer energy group structure required (up to 33 groups), the lower cross sections values, or the usual hexagonal geometry design, have a big impact in the applicability of the ACMFD method, as it will be discussed in this section.

In order to assess the ACMFD method, assembly calculations were performed, using specifications provided by the "Working Horses" of the ESFR core [10].

### 4.1. Limitation of the ACMFD method when dealing in 3D with many energy groups

First, we calculated with ANDES code in 33 energy groups a 2-D fuel-subassembly with reflective boundary conditions and satisfactory results were obtained. However, some difficulties were encountered when performing the fuel-subassembly calculation in 3-D adding the axial reflectors. The ACMFD method gave rise to negative fluxes and fission source values during the convergence process. After a rigorous examination, we found some anomalies concerning the decoupling of the multigroup diffusion equation.

According to the formulation of the ACMFD method, a relationship between the flux at the interface in terms of the average flux at the adjacent node and of the current at the same interface is established. This relation comes from the analytic solution of equation (4), which in 1D is expression (5), and where $p_m(x)$ is a particular solution of the heterogeneous equation with a transverse leakage source.

$$\psi_m(x) = A_m e^{+\alpha_m x} + B_m e^{-\alpha_m x} + p_m(x) \;; \qquad \alpha_m = \sqrt{\lambda_m} \tag{5}$$

Determining the constants $A_m$ and $B_m$ from the values of flux and current on interfaces:

$$\psi_m(\mp\frac{H}{2}) - p_m(\mp\frac{H}{2}) = C_m^f[\overline{\psi}_m - \overline{p}_m] \pm C_m^j \frac{H}{2}\left[J_m(\mp\frac{H}{2}) + p'_m(\mp\frac{H}{2})\right] \tag{6}$$

Where $C^f$ and $C^j$ are constants for every mode and depend only on the eigenvalue, the cross sections, and the nodal width over the considered direction.

$$C_m^f = \frac{2\alpha_m H}{e^{+\alpha_m H} - e^{-\alpha_m H}} \;; \qquad C_m^f = \frac{e^{+\alpha_m H} + e^{-\alpha_m H} - 2}{e^{+\alpha_m H} - e^{-\alpha_m H}} \cdot \frac{2}{\alpha_m H} \tag{7}$$

Finally, transforming from the modal fluxes to the physical group fluxes, using (3), we obtain:

$$|\phi_g(\mp\frac{H}{2})\rangle = A^f\,|\overline{\phi}_g\rangle \pm \frac{H}{2} A^j D_g^{-1}\,|J_g(\mp\frac{H}{2})\rangle - R^{-1}\,|T_m(\mp\frac{H}{2})\rangle \tag{8}$$

$$A^f = R^{-1} C^f R; \qquad A^j = R^{-1} C^j R \tag{9}$$

After examining the relations in (7), it is clear that the finer the mesh is, the closer to 1 those coefficients have to be, since:

$$lim(H \to 0) C_m^f = 1 \; ; \quad lim(H \to 0) C_m^j = 1 \tag{10}$$

Indeed, both coefficients were verified to tend to 1 as the mesh gets finer in ANDES. However, when we analyzed the matrices $A^f$ and $A^j$, it happened that they do not tend to the identity as it should have been from (9), taking into account that both $C^f$ and $C^j$ are almost 1. This fact led us to a more accurate study of the multi-group diffusion matrix and the procedure to calculate their eigenvalues and eigenvectors, particularly for reflector material nodes (axial blankets, gas plenums and radial reflectors).

As it is usual in fast reactor calculations not to consider up-scattering, the matrix $\boldsymbol{A}$ in equation (1) corresponding to a non-fissile material is lower triangular, which means that eigenvalues might be easily extracted from the main diagonal. However, when a simple check is performed to the eigenvector matrix $\boldsymbol{R}$, it is noticed that it does not verify the relations (11) nor (12).

$$R \cdot R^{-1} = I \tag{11}$$

$$A = R^{-1} [\lambda_m]_{diag} R \tag{12}$$

That is, the calculation method of the inverse matrix is not working properly. Besides, after examining their eigenvalues it is concluded that some of them are close to one another. This deteriorates the conditioning number of their associated eigenvectors, which cannot be well determined. Therefore, since fast reactor calculations typically involve at least 33 energy groups, the multigroup diffusion matrices generated do not present optimal numerical properties regarding their conditioning. This fact has proved to be relevant in the non-fissile materials.

### 4.2. Implementation of the FMFD diffusion scheme in ANDES

Since a limitation in the application of ACMFD method to the 33 group mini-core has been found, a Fine Mesh Finite Difference (FMFD) scheme has been successfully implemented in ANDES code. It can be used for non –fissile material nodes –where ACMFD method fails– until new numerical methods are implemented and tested.

When comparing the half-node ACMFD formula (13) with the Fick's Law (14) the former coincides with the latter if the matrices $A^f$ and $A^j$ are the identity.

$$|J_g(\mp\frac{H}{2})\rangle = \mp D_g A^{j-1} \frac{A^f |\bar{\phi}_g\rangle - |\bar{\phi}_g(\mp\frac{H}{2})\rangle}{H/2} \tag{13}$$

$$|J_g(\mp\frac{H}{2})\rangle = \mp D_g \frac{|\bar{\phi}_g\rangle - |\bar{\phi}_g(\mp\frac{H}{2})\rangle}{H/2} \quad (14)$$

Therefore, forcing the matrices to be the identity and removing the traverse leakage effect, we achieve the implementation of the Finite Mesh Finite Difference diffusion approach in ANDES.

## 5. RESULTS

In order to verify the performance of ANDES two studies have been carried out. First, a 3D mini-core model previously calculated with ERANOS was used as a home-made benchmark to compare with the FMFD diffusion solver implemented in ANDES. Second, a NEA benchmark for a small 3D FBR was employed to verify the performance of ANDES code with the ACMFD method in a few-energy-groups structure (4 groups).

### 5.1. 3D mini-core home-made benchmark with ERANOS

A 3D mini-core was modeled from the geometry and material composition specifications of the "Working Horses" document of the ESFR project [10] as shown in Fig.2. It consists on a control rod CSD type sub-assembly surrounded by a ring of fuel sub-assemblies corresponding to the inner region of the oxide core from the ESFR. A layer of reflector assemblies is placed in the periphery, surrounding the fuel assemblies. The axial description, from the specifications of the ESFR core, consists in a fission gas plenum with a lower axial blanket bellow the active zone and a small thin layer of fission gas plenum and another axial plenum over the active zone, as shown in Fig.2b. The control rod is considered withdrawn for the simulation.

Calculations were performed in 33 energy groups at HFP conditions, assuming a thermal power of 50MW.

ERANOS system can perform both diffusion and transport calculations, and both options were used to benchmark the performance of ANDES code using the FMFD scheme.

In the following, we present the results of ANDES without radial refinement using just 1 node per triangle –6 nodes per assembly– (ANDES 1), and refining to 4 nodes per triangle –24 nodes per assembly– (ANDES 2). Additionally, a third calculation (ANDES 3) was performed with ANDES in two consecutive steps: first using the FMFD diffusion approach and afterwards using the obtained solution to initialize a second ANDES calculation where the FMFD scheme is only used in the non-fissile zones while the ACMFD method is used in the fissile zones. A mesh refinement of 4 nodes per triangle was taken in this last calculation.

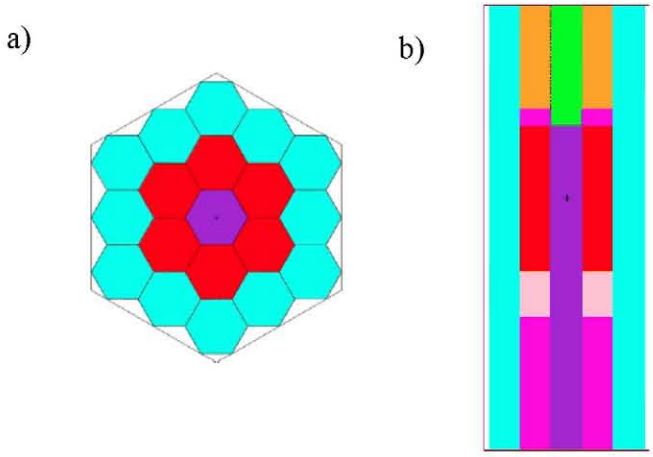


**Figure 2. Mini-core description: a) Radial & b) Axial**

**Table II. K-eff for ERANOS and ANDES.**

| | ERANOS-DIF | ERANOS-TR | ANDES(1) | ANDES(2) | ANDES(3) |
|---|---|---|---|---|---|
| **K-eff** | 0.4955 | 0.5427 | 0.6522 | 0.6420 | 0.6052 |
| **reactivity difference (pcm)** | -17544 | reference | 30946 | 28493 | 19018 |

Table II shows k-eff values computed by ERANOS and ANDES codes. Large discrepancies are seen between ERANOS diffusion and transport solutions. When using ANDES, deviations with respect to transport solution are also very large, showing that conventional diffusion theory is not reliable for fast reactors; consequently, discontinuity factors need to be used in order to obtain a corrected diffusion solution close to the transport one. Comparing the ANDES calculations, it can be seen that the finer the radial discretization is, the smaller the discrepancies are. The lowest discrepancies are observed when using the ACMFD method in the fissile zone (ANDES 3).

Fig. 3 represents the comparison of the axial power distribution between ERANOS –with both diffusion and transport modes- and ANDES. The axial profile of the power distribution shows a good agreement between both codes.

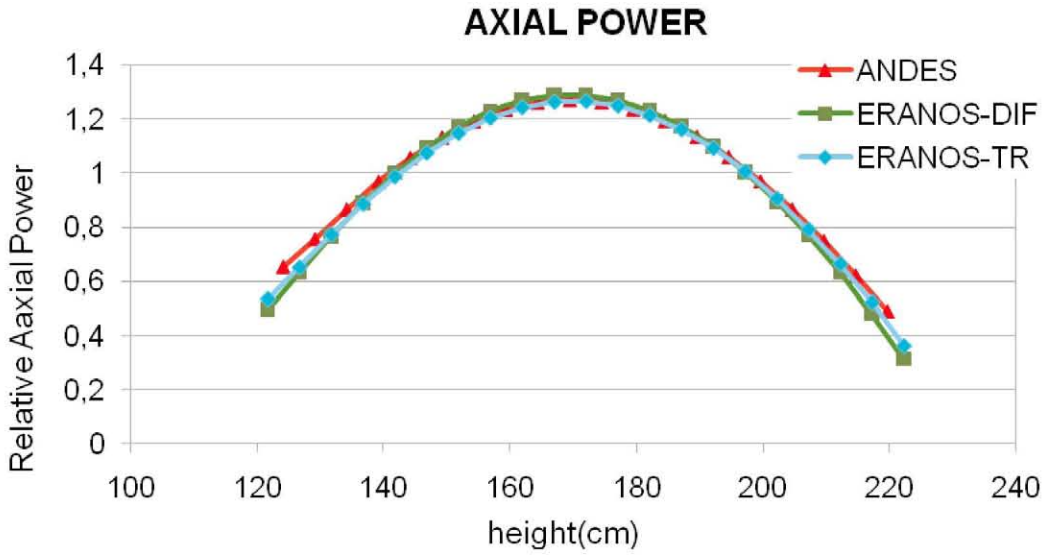


**Figure 3. Axial Power distribution by ERANOS and ANDES.**

Consequently, the FMFD diffusion solver implemented in ANDES works acceptably well in 33 groups, but further efforts must be carried out in order to be able to apply ACMFD solver also for non-fissile materials, as well as to improve ANDES performance by using interface discontinuity factors.

### 5.2. 3D small FBR benchmark in 4 groups

In order to assess the performance of ANDES while dealing with a few-energy-groups structure and thus eliminating the problem concerning the ill-conditioning of the diffusion matrices in many energy-groups, a NEA benchmark in 4 energy groups was computed [11]. The core model chosen was proposed by L. Broeders and E. Kiefhaber of KFK, Germany, and is a model of the KNK-II core, being the geometry hexagonal-Z as shown in Fig. 4.

We study here the case where the control rods are completely withdrawn from the active zone of the core and we aim to compare the results of k-eff between ANDES and the contributors to the benchmark, all of them using transport codes (benchmark results are shown in Fig. 5).

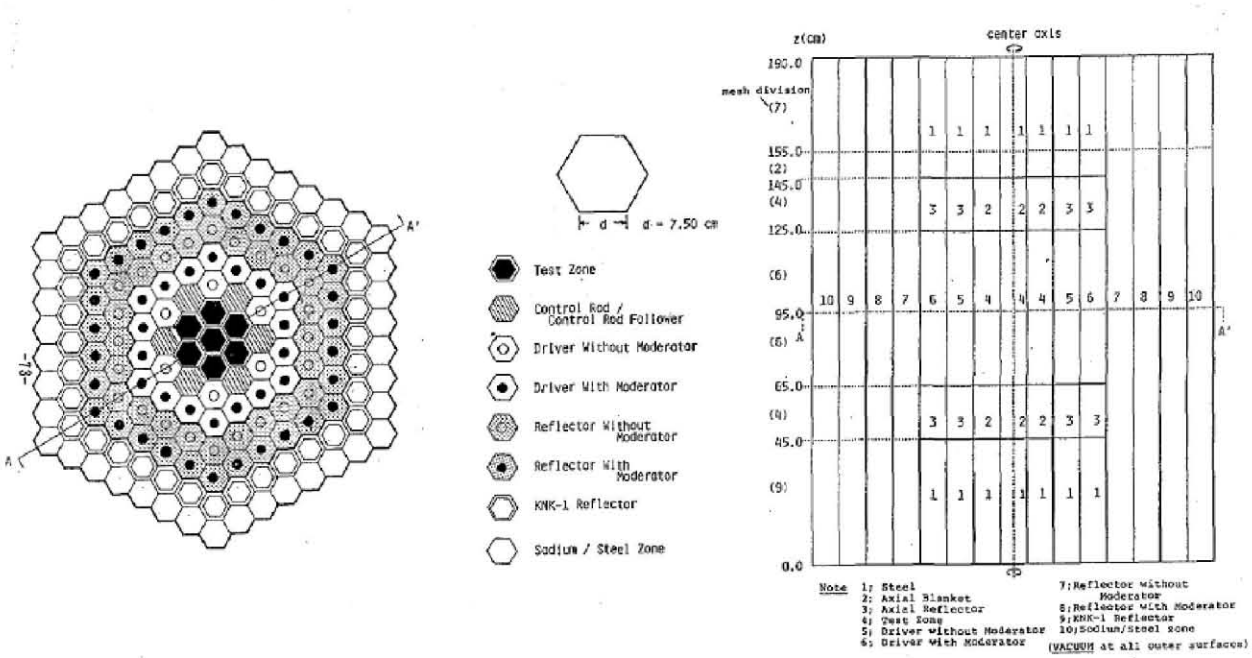


**Figure 4. 3-D Small FBR model description**

Several calculations have been performed with ANDES code using its inherent ACMFD method in both hexagonal and Cartesian geometry, and k-eff results are shown in Table III.

**Table III. K-eff of ANDES in different options**

| | Hex-ACMFD n=1 | Hex-ACMFD n=2 | Cart-ACMFD n=1 |
|---|---|---|---|
| K-EFF | 1.07567 | 1.07518 | 1.07652 |

ANDES calculations did converge to the desired level during execution. Comparing the results from the hexagonal configuration with its analogous Cartesian configuration, a very good agreement is observed. It points out that the traverse leakage interpolation in triangular geometry is successfully implemented even though the procedures required were much more complex than for Cartesian geometry. Moreover, the mesh refinement (n=2, 24 triangles per assembly) confirms that the solution is well converged.

The ACMFD method provides acceptable results. However, when compared with the ones given by the benchmark participants, still significant discrepancies can be seen as expected since ANDES is a diffusion solver and the benchmark participants contributed with transport solvers.

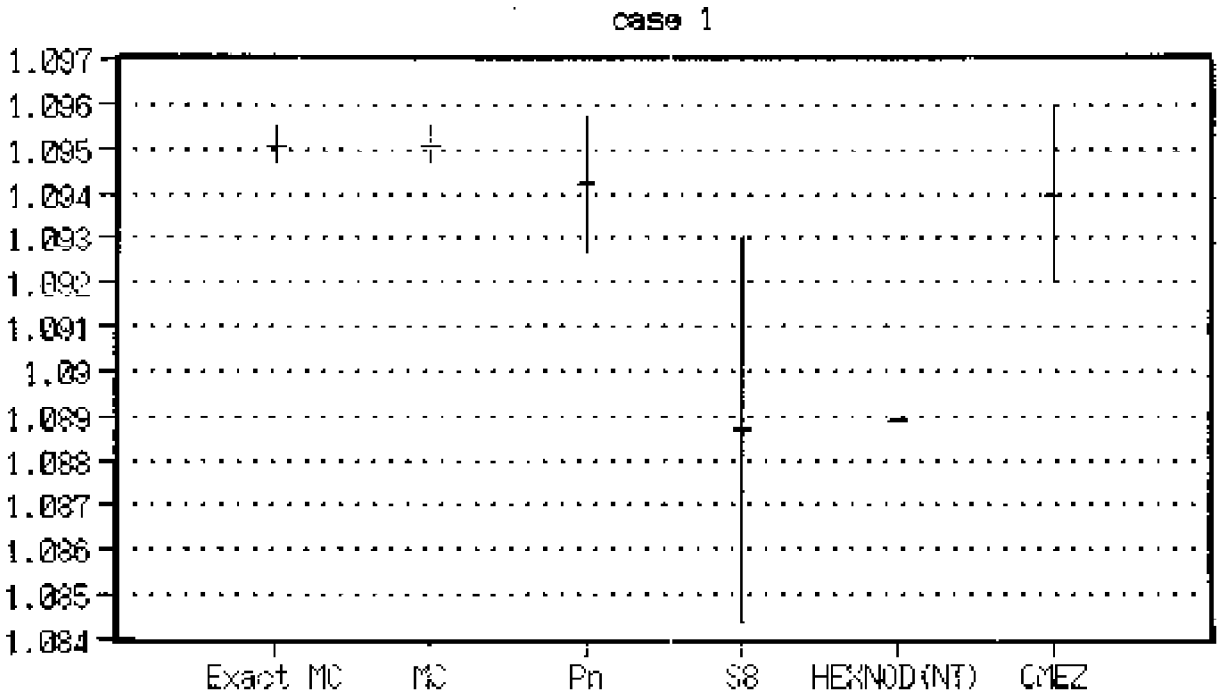


**Figure 5. Average k-eff values for different transport codes**

## 6. CONCLUSIONS

At UPM an extensive work is being performed in order to extend our in-house code system for pin-by-pin and nodal coupled NK-TH simulations to sodium fast reactors. This paper discusses the first steps towards the application of the nodal diffusion solver ANDES.

When applying ANDES to fast reactors, some limitations have been encountered. Concerning the fine energy group structure required in fast reactors calculations, it has been demonstrated that the multigroup diffusion matrices corresponding to the non-fissile materials do not present optimal numerical properties with respect to their conditioning when using 33 energy groups. Thus, the ACMFD solver does not fully converge in these situations. Then, a FMFD diffusion approach was successfully implemented in ANDES, avoiding matrix diagonalization. A mixed solution was also tried out where the ACMFD scheme is only applied to the fissile zones and the FMFD elsewhere, giving more accurate results than the FMFD method. Further improvements are in progress to overcome those ill-conditioned problems and then apply ACMFD scheme also in non-fissile materials.

On the other hand, when a few energy groups structure is employed and thus, the related conditioning problems of the multigroup diffusion matrix do not exist, the ANDES solver has proved to work satisfactorily well.

Finally, comparison of ANDES and transport solutions for 3D fast reactors show that adequate interface discontinuity factors must be used so that corrected diffusion solution can produce more accurate results, while maintaining low computational cost.

## ACKNOWLEDGMENTS

*This work is especially dedicated to the memory of José María Aragonés. His constant work and restless dedication will always inspire our work and progress.*

The research leading to these results has received funding from the European Community's Seventh Framework Program [*FP7/2007-2013*] under *grant agreement* n° 232658.

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